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# Trace formula for systems with spin from the coherent state propagator

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We present a detailed derivation of the trace formula for a general Hamiltonian with two degrees of freedom where one of them is canonical and the other a spin. Our derivation starts from the semiclassical formula for the propagator in a basis formed by the product of a canonical and a spin coherent states and is valid in the limit $\hbar \to 0$, $j \to \infty$ with $j\hbar$ constant. The trace formula, obtained by taking the trace and the Fourier transform of the coherent state propagator, is compared to others found in the literature. © *2007 American Institute of Physics.* [DOI: 10.1063/1.2806487]

## I. INTRODUCTION

Since the beginning of the last century, with the development of quantum mechanics, much work has been done on the study of its connection with classical mechanics. This investigation, generally known as *semiclassical methods*, became a rich field on its own, having been motivated both by conceptual and practical reasons. The conceptual motivations are closely related to the *correspondence principle*, which basically says that quantum mechanics must reproduce predictions to the classical theory when typical actions of the system are much larger than Planck's constant $\hbar$. Keeping in mind this philosophical principle, one hopes to establish and understand relations between quantal and classical objects in the appropriate limit. The practical motivations, on the other hand, hinge on the fact that semiclassical formulas provide approximations for the corresponding quantum quantities involving only classical ingredients. These, for many systems of interest, are easier to calculate than the exact quantal counterparts and may provide accurate approximations.

In spite of the early development of the semiclassical theory, nonintegrable classical systems were only properly dealt with at the end of the 1960s. As the pioneering quantization rules of Bohr-Sommerfeld[1] and Einstein-Brillouin-Keller[2] depend on the calculation of actions over irreducible circuits, their application to nonintegrable systems is not possible. Therefore, for classically chaotic systems, there was no way of extracting quantum information from classical functions. The Gutzwiller trace formula[3] filled this gap for totally chaotic systems, associating the periodic orbits of the corresponding classical system with the energy level density (see Sec. II).

Gutzwiller's original work, however, did not consider spin degrees of freedom. A number of attempts to find a semiclassical trace formula for systems with spin were made, as reviewed in a recent paper by Amman and Brack.[4] There, the works of Littlejohn and Flynn,[5] Frisk and Guhr,[6]

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and Bolte and Keppeler[7] are discussed in detail. In Ref. 4, the authors also mention a general trace formula obtained by Pletyukhov *et al.*[8] for Hamiltonians linear in the spin variable, $\hat{H}=\hat{H}_0(\hat{\mathbf{q}},\hat{\mathbf{p}})+\hbar\hat{\mathbf{s}}\cdot\hat{\mathbf{C}}(\hat{\mathbf{q}},\hat{\mathbf{p}})$. Since this work generalizes the former ones, it shall be used in the discussion of our result. Apart from these works, dealing with canonical and spin variables simultaneously, in Ref. 9 the authors considered the semiclassical quantization of systems with *only* spin degrees of freedom.

In this paper we present a detailed derivation of the semiclassical limit of the quantum density of energy levels for *general* systems representing a spatial degree of freedom and a spin of magnitude $j$. Systems in this category include those involving spin-orbit interactions and the so called spin-boson model, which has been intensively investigated in the context of quantum dissipation.[10,11] The calculation is performed taking the limit where $\hbar \to 0$ and $j\to\infty$, with $j\hbar$ constant in a basis which is the product of spin and canonical coherent states. The starting point of our derivation is the semiclassical propagator in this representation derived in Ref. 12. The special case $j=1/2$ will also be discussed.

Our final result resembles that of Pletyukhov *et al.*[8] Our derivation, however, is valid for general Hamiltonians. Besides, Pletyukhov *et al.* started directly from a partition function containing spin and spatial degrees of freedom, following a route similar to that of Sugita[13] in the study of quadratic canonical Hamiltonians, which avoids the calculation of the propagator. Both works make use of a joint phase space, composed by canonical and spin degrees of freedom, where the classical dynamics takes place. The connection between the two formulas is discussed in Sec. VI.

The paper is organized as follows. In the next three sections we present some preliminary concepts that are useful to understand our derivation. In Secs. II and III, we review the basic formulas connecting the energy level density with the propagator and the representations of canonical and spin coherent states. In Sec. IV, we present the semiclassical propagator used as our starting point. The derivation of the spin trace formula is outlined in Sec. V. Finally, we present our final remarks in Sec. VI.

## II. PRELIMINARY DISCUSSION

In this section we review basic quantum mechanics expressions involved in Gutzwiller's derivation of the semiclassical density of states. However, instead of adopting right away the coordinate basis $\{|q\rangle\}$ for the propagator, we consider an arbitrary basis labeled by a (possibly complex) number $b$, $\{|b\rangle\}$.

For a time-independent Hamitonian $\hat{H}$, the matrix element of the time evolution operator, or quantum propagator, is given by

$$K(b''^{*},b',T) \equiv \langle b''|e^{-i\hat{H}T/\hbar}|b'\rangle = \sum_{n=0}^{\infty}\langle b''|n\rangle\langle n|b'\rangle e^{-iE_nT/\hbar}, \tag{1}$$

where $\{|n\rangle\}$ are the eigenstates of $\hat{H}$, with eigenvalues $E_n$. Taking the Fourier transform of Eq. (1) we obtain Green's function

$$G(b''^{*},b',E+i\epsilon) \equiv \frac{1}{i\hbar}\int_0^{\infty} K(b''^{*},b',T)e^{(i/\hbar)(E+i\epsilon)T}dT = \sum_{n=0}^{\infty}\frac{\langle b''|n\rangle\langle n|b'\rangle}{E-E_n+i\epsilon}, \tag{2}$$

where $\epsilon$ is a small real parameter needed to handle the singularity of the integral. The function $G(b''^{*},b',E+i\epsilon)$ can also be understood as matrix elements of the operator $(E+i\epsilon-\hat{H})^{-1}$. Taking its trace we get

$$g(E+i\epsilon)=\int G(b^*,b,E+i\epsilon)d\mu(b^*,b)=\sum_{n=0}^{\infty}\frac{1}{E-E_n+i\epsilon}, \tag{3}$$

where the measure $d\mu(b^*,b)$ ensures the completeness of the basis $\{|b\rangle\}$, including a possible normalization factor. Writing each term in the sum of Eq. (3) as

$$\frac{1}{E-E_n+i\epsilon}=\left[\frac{E-E_n}{(E-E_n)^2+\epsilon^2}-\frac{i\epsilon}{(E-E_n)^2+\epsilon^2}\right] \tag{4}$$

and taking the limit $\epsilon\to 0$, we identify the quantum density of energy levels,

$$n(E)\equiv\sum_{n=0}^{\infty}\delta(E-E_n)=-\frac{1}{\pi}\,\mathrm{Im}[g(E)]. \tag{5}$$

This relation between the density of states and the trace of Green's function is the key to Gutzwiller's work. Working in the position representation, he started from the Van-Vleck semiclassical propagator $K_{\mathrm{VV}}(q'',q',T)$ and performed the Fourier transform and the trace by the stationary phase method. The Van-Vleck propagator is a semiclassical formula for $\langle q''|e^{-i\hat{H}T/\hbar}|q'\rangle$, written exclusively in terms of classical trajectories of a Hamiltonian function $H$, the Weyl symbol of $\hat{H}$, starting at $q'$ and ending at $q''$ after a time $T$. In the semiclassical limit, the Fourier transform (2) of $K_{\mathrm{VV}}(q'',q',T)$ selects from these trajectories those restricted to energy $E$, independently of $T$, and sums their contributions. Finally, the trace (3) selects only periodic orbits. Performing all calculations, and for the case of chaotic systems, the semiclassical density of states takes the form

$$n_{\mathrm{sc}}(E)=n_0(E)+\sum_{\mathrm{per.orb.}}\frac{1}{\pi\hbar}\frac{T_0}{\sqrt{|\det(\mathrm{M}-\mathrm{I})|}}\cos\left\{\frac{1}{\hbar}S(E)-\frac{\pi}{2}\sigma\right\}, \tag{6}$$

where $n_0$ is a smooth term resulting from the contributions of trajectories with zero period. The sum runs over all periodic orbits with energy $E$. The function $S(E)$ is Hamilton's action of the periodic orbit and $T_0$ its primitive period. Finally the matrix $M$ is the stability (or monodromy) matrix and $\sigma$ the Maslov index.

## III. COHERENT STATES

Coherent states have been widely used in many areas of physics such as quantum optics and atomic and nuclear physics. These states also play an important role in the study of the semiclassical limit of the quantum mechanics. A number of books and review articles have been written on this subject, as, for example, Refs. [14–16]. In this paper we are particularly interested in two kinds of coherent states, the *canonical* and the *spin* coherent states, as termed by Klauder and Skagerstam.[14]

A canonical coherent state $|z\rangle$ is obtained from the application of the Weyl operator $\exp\{z\hat{a}^\dagger-\frac{1}{2}|z|^2\}$ on the ground state of a harmonic oscillator of mass $m$ and frequency $\omega$, namely,

$$|z\rangle=\exp\{z\hat{a}^\dagger-\tfrac{1}{2}|z|^2\}|0\rangle. \tag{7}$$

The complex number $z$ labeling the canonical coherent state is eigenvalue of the annihilation operator $\hat{a}$ associated with the eigenvector $|z\rangle$. Writing $z$ as

$$z=\frac{1}{\sqrt{2}}\left(\frac{\bar{q}}{b_z}+i\frac{\bar{p}}{c_z}\right), \tag{8}$$

we may identify $\bar{q}$ and $\bar{p}$, respectively, as the average values of the position $\hat{q}$ and momentum $\hat{p}$ operators. The numbers $b_z=\sqrt{\hbar/(m\omega)}$ and $c_z=\sqrt{m\hbar\omega}$ are the dispersion along the position and momentum axes, respectively, satisfying $b_z c_z=\hbar$. This last feature characterizes the states $|z\rangle$ as minimum uncertainty states. The resolution of unit and the overlap between two such states are given by

$$\int \frac{dz^{(R)}dz^{(I)}}{\pi}|z\rangle\langle z| \equiv 1_z, \quad \langle z_1|z_2\rangle = \exp\{-\tfrac{1}{2}|z_1|^2 + z_1^* z_2 - \tfrac{1}{2}|z_2|^2\}, \tag{9}$$

where $z^{(R)}$ and $z^{(I)}$ are, respectively, the real and the imaginary part of $z$.

From the group theory point of view, canonical coherent states belong to the Heisenberg-Weyl group. Spin coherent states $|s\rangle$ can also be defined in analogy to the canonical case. For a $(2j+1)$-dimensional spin multiplet $|s\rangle$ is given by

$$|s\rangle = \frac{\exp\{s\hat{J}_+\}}{(1+|s|^2)^j}|-j\rangle, \tag{10}$$

where the denominator accounts for the normalization. The label $s$ is a complex number, $\hat{J}_+$ is the raising spin operator, and $|-j\rangle$ is the extremal eigeinstate of $\hat{J}_3$ with eingenvalue $-j$. Completeness and overlap relations are given by

$$\frac{2j+1}{\pi}\int \frac{ds^{(R)}ds^{(I)}}{(1+|s|^2)^2}|s\rangle\langle s| \equiv 1_s, \quad \langle s_1|s_2\rangle = \frac{(1+s_1^* s_2)^{2j}}{(1+|s_1|^2)^j(1+|s_2|^2)^j}, \tag{11}$$

where $s^{(R)}$ and $s^{(I)}$ are, respectively, the real and the imaginary part of $s$. The integrals above as well as those of Eq. (9) run from $-\infty$ to $+\infty$.

Determining the physical content of the label $s$ is more involved than the corresponding task for its counterpart $z$, and it is better understood in terms of Bloch's sphere. The complex plane defined by $s=s^{(R)}+is^{(I)}$ can be seen as the plane where a sphere (Bloch's sphere) of radius of 1 is stereographically projected. We define such a plane as the plane that divides the sphere in north and south hemispheres. Considering a projection performed from the north pole, the south pole corresponds to the origin of the plane and the north pole to infinity. The modulus $|s|$ depends just on the angle $\alpha$ measured from the north pole, $|s|=\tan\alpha$. However, it is more convenient to write $|s|$ as function of $\theta$, the polar angle in spherical coordinates, leading to $|s|=\cot(\theta/2)$. Therefore, to a given unit vector $\mathbf{n}=(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)\equiv(n_1,n_2,n_3)$ in the Bloch sphere, where $\theta$ and $\phi$ are the spherical coordinates, we associate $s=|s|e^{-i\phi}$, or explicitly,

$$|s| = \cot(\theta/2), \quad s^{(R)} = \cot(\theta/2)\cos\phi, \quad s^{(I)} = -\cot(\theta/2)\sin\phi. \tag{12}$$

Using Eqs. (10) and (12), and the commutation relations of the angular momentum, we find

$$\langle\hat{\mathbf{J}}\rangle = j\mathbf{n}, \quad \langle\{\Delta\hat{J}_k, \Delta\hat{J}_l\}\rangle = j(\delta_{k,l}-n_k)(\delta_{k,l}+n_l),$$

$$\langle\hat{J}_k^2\rangle = j\left(j-\frac{1}{2}\right)n_k^2 + \frac{j}{2}, \quad \langle(\Delta\hat{J}_k)^2\rangle = \frac{j}{2}(1-n_k^2), \tag{13}$$

where we have defined the operator $\Delta\hat{J}_k \equiv \hat{J}_k - \langle\hat{J}_k\rangle$ and $k,l=1,2,3$. The average in the last equations is taken over the coherent state $|s\rangle$, and the brackets $\{\cdot,\cdot\}$ stand for the anticommutator. Applying these results to the uncertainty relation[17] $\langle\Delta\hat{A}^2\rangle\langle\Delta\hat{B}^2\rangle \geqslant \frac{1}{4}|\langle[\hat{A},\hat{B}]\rangle|^2 + \frac{1}{4}|\langle\{\Delta\hat{A},\Delta\hat{B}\}\rangle|^2$; it can be shown that $|s\rangle$ are minimun uncertainty states because they saturate such a relation.

## IV. SEMICLASSICAL PROPAGATOR FOR SYSTEMS WITH SPIN

Semiclassical approximations for the quantum propagator (1) in the coherent state representation were first performed by Klauder,[18,19] who considered both spin and canonical coherent states. However, the semiclassical formula missed a term that was derived only later by

Kochetov[20] and Baranger *et al.*,[21] for canonical states (see Ref. 22 for a recent review), and by Solari,[23] Vieira and Sacramento,[24] Kochetov,[25] and Stone *et al.*,[26] for spin states.

Results for problems involving spin and canonical degrees of freedom were considered only for particular cases (see Ref. 27). Only recently a general semiclassical formula for the propagator $\langle z'',s''|e^{-i\hat{H}T/\hbar}|z',s'\rangle$ was obtained.[12] The result is

$$K_{\text{sc}}(z''^*,s''^*,z',s',T)=\sum_{\text{c.t.}}\sqrt{\frac{1+U''V''}{1+U'V'}\frac{1}{\det M_{bb}}}e^{(i/\hbar)(\mathcal{S}+\mathcal{G})-\Lambda}. \tag{14}$$

The right hand side of this equation depends only on *complex* classical trajectories governed by the average Hamiltonian $\tilde{H}\equiv\langle z,s|\hat{H}|z,s\rangle$. In terms of the auxiliary variables $u$, $v$, $U$, and $V$, the Hamilton equations are

$$\frac{\partial\tilde{H}}{\partial u}=-i\hbar\dot{v},\quad \frac{\partial\tilde{H}}{\partial U}=\frac{-2ij\hbar\dot{V}}{(1+UV)^2},\quad \frac{\partial\tilde{H}}{\partial v}=i\hbar\dot{u},\quad \frac{\partial\tilde{H}}{\partial V}=\frac{2ij\hbar\dot{U}}{(1+UV)^2}, \tag{15}$$

where $\tilde{H}$ is defined by $\tilde{H}(u,U,v,V)=\tilde{H}(z,s,z^*,s^*)\equiv\langle z,s|\hat{H}|z,s\rangle$. Notice that this equality implicitly defines the new variables through the substitution of $z$, $s$, $z^*$, and $s^*$ by, respectively, $u$, $U$, $v$, and $V$. In addition, trajectories contributing to (14) must satisfy the boundary conditions

$$u'=z',\quad v''=z''^*,\quad U'=s',\quad \text{and } V''=s''^*, \tag{16}$$

where we have used the usual notation that a single (double) prime stands for initial (final) time. The sum in Eq. (14) is over all trajectories described by Eqs. (15) and (16).

The complex action $\mathcal{S}=\mathcal{S}(z''^*,s''^*,z',s',T)$ and the function $\mathcal{G}=\mathcal{G}(z''^*,s''^*,z',s',T)$, in Eq. (14), are explicitly written as

$$\mathcal{S}=\int_0^T\left\{\frac{i\hbar}{2}(\dot{u}v-\dot{v}u)-i\hbar j\left(\frac{U\dot{V}-V\dot{U}}{1+UV}\right)-\tilde{H}\right\}dt-i\hbar\tilde{\Lambda},$$

$$\mathcal{G}=\frac{1}{2}\int_0^T\left\{\frac{\partial^2\tilde{H}}{\partial v\,\partial u}+\frac{1}{2}\left[\frac{\partial}{\partial V}\frac{(1+VU)^2}{2j}\frac{\partial\tilde{H}}{\partial U}+\frac{\partial}{\partial U}\frac{(1+VU)^2}{2j}\frac{\partial\tilde{H}}{\partial V}\right]\right\}dt. \tag{17}$$

Notice that the function $\mathcal{G}$ contains the Solari-Kochetov phase,[23–26] plus its canonical counterpart (the first term of the integral). In addition, $\Lambda$, that accounts for the normalization, and $\tilde{\Lambda}$, from Eq. (17), are given by

$$\Lambda=\tfrac{1}{2}(|u'|^2+|v''|^2)+j\ln[(1+|U'|^2)(1+|V''|^2)],$$

$$\tilde{\Lambda}=\tfrac{1}{2}(u'v'+u''v'')+j\ln[(1+U'V')(1+U''V'')], \tag{18}$$

and $M_{bb}$ is a $2\times2$ block of the stability matrix $M$, that propagates small displacements around the complex classical orbit,

$$\begin{pmatrix}\delta u''\\ \delta U''\\ \delta v''\\ \delta V''\end{pmatrix}=\begin{pmatrix}M_{aa} & M_{ab}\\ M_{ba} & M_{bb}\end{pmatrix}\begin{pmatrix}\delta u'\\ \delta U'\\ \delta v'\\ \delta V'\end{pmatrix}. \tag{19}$$

The phase of $\det M_{bb}$ plays a similar role to the Maslov phase in the coordinate propagator. Because of the square root in Eq. (14), we must follow it over time and add, after each complete turn, a phase of $-\pi$ to the propagator.

Finally, we write down the useful relations

$$\frac{\partial \mathcal{S}}{\partial u'} = -i\hbar v', \quad \frac{\partial \mathcal{S}}{\partial U'} = \frac{-2ij\hbar V'}{1+U'V'}, \quad \frac{\partial \mathcal{S}}{\partial v''} = -i\hbar u'', \quad \frac{\partial \mathcal{S}}{\partial V''} = \frac{-2ij\hbar U''}{1+U''V''}, \tag{20}$$

and $\partial \mathcal{S}/\partial T = -\tilde{H}(u',U',v',V') = -\tilde{H}(u'',U'',v'',V'')$.

## V. SEMICLASSICAL TRACE FORMULA FOR SYSTEMS WITH SPIN

Our approach to derive the trace formula differs from that presented in Sec. II in that we invert the steps given by Eqs. (2) and (3), namely, we first take the trace of the propagator, and then its Fourier transform. The calculation proceeds as follows. First we calculate trace of the propagator using the steepest descent method and show that the trajectories that contribute in this approximation are real and periodic. In order to calculate the contribution of each trajectory to the trace, we introduce a special set of canonical variables in terms of which the stability matrix assumes a particularly simple form. Finally, we Fourier transform the trace obtaining the desired trace formula.

### A. The trace of the propagator

To find the semiclassical trace of the propagator, we must perform the integral

$$K_{\rm sc}(T) = \frac{2j+1}{\pi^2} \int K_{\rm sc}(v'',V'',u',U',T) \frac{dz^{(R)}dz^{(I)}ds^{(R)}ds^{(I)}}{(1+|s|^2)^2}, \tag{21}$$

where the labels of the bra $\langle z''s''|$ and the ket $|z's'\rangle$ defining the propagator must be the same. Therefore, the trajectories entering in $K_{\rm sc}(v'',V'',u',U',T)$ must satisfy the boundary conditions

$$u' = z = z^{(R)} + iz^{(I)}, \quad U' = s = s^{(R)} + is^{(I)},$$

$$v'' = z^* = z^{(R)} - iz^{(I)}, \quad V'' = s^* = s^{(R)} - is^{(I)}. \tag{22}$$

We emphasize that, in spite of the conditions (22), trajectories are still complex, since $v'$ is not necessarily $z^*$, the same happening with $u''$ and $z$, $V'$ and $s^*$, and $U''$ and $s$. The integral (21) means that all trajectories with period $T$ and satisfying Eqs. (15) and (22), and for all values of $z$ and $s$, contribute to $K_{\rm sc}(T)$.

In the semiclassical limit $\hbar \to 0$, $j \to \infty$, with $j\hbar$ constant, we can apply the steepest descent method in order to select the relevant trajectories to integral (21). However, it is convenient to use Jacobian $dz^{(R)}dz^{(I)}ds^{(R)}ds^{(I)} \to -\frac{1}{4}du'dv''dU'dV''$ and also Eq. (14) to rewrite (21) as

$$K_{\rm sc}(T) = \frac{2j+1}{-4\pi^2} \int \sqrt{\frac{1+U''V''}{1+U'V'}\frac{1}{\det M_{bb}}} e^{(i/\hbar)F(v'',V'',u',U',T)} \frac{du'dv''dU'dV''}{(1+U'V'')^2}, \tag{23}$$

where $F = \mathcal{S} + \mathcal{G} + i\hbar(u'v'' + 2j\ln[1+U'V''])$. The saddle points of (23) are solutions of

$$\frac{\partial F}{\partial u'} = \frac{\partial F}{\partial v''} = \frac{\partial F}{\partial U'} = \frac{\partial F}{\partial V''} = 0, \tag{24}$$

which, using relations (20) and disregarding derivatives of $\mathcal{G}$ as usual (see Ref. 21), produces

$$v' = v'' \equiv \bar{z}^*, \quad u'' = u' \equiv \bar{z}, \quad V' = V'' \equiv \bar{s}^*, \quad U'' = U' \equiv \bar{s}. \tag{25}$$

Equations (25) determine the values of the variables of integration whose vicinity is relevant to the calculation of $K_{\rm sc}(T)$. These special points correspond to periodic trajectories of period $T$. The periodicity condition is equivalent to saying that $u$ and $v$ (and also $U$ and $V$) are complex conjugate each other, which assures that only *real* periodic trajectories must be considered. Each set of points $(\bar{z},\bar{z}^*,\bar{s},\bar{s}^*)$ that gives origin to a periodic orbit with period $T$, independent of the value of its energy, is therefore a saddle point of the integral (23). In addition, as we shall see in the following, trajectories lying the vicinity of the real orbit shall be considered in the calculation of the second order corrections. Such trajectories are still complex and are specified by the deviations $(\delta u', \delta v'', \delta U', \delta V'')$ around the point $(u'=\bar{z}, v''=\bar{z}^*, U'=\bar{s}, V''=\bar{s}^*)$ of the periodic orbit.

### B. Expansion around periodic orbits: Preliminary discussion

Consider, for the sake of simplicity, that there is just one trajectory with period $T$. Each point along this orbit is a saddle point of (23). Therefore, summing over critical points means, in particular, to integrate along the periodic orbit. In addition, the saddle point method demands the evaluation of the contribution of the vicinity of each saddle point. This, in turn, means that we should calculate the contribution of paths belonging to an infinitesimal phase space tube centered at the periodic orbit.[3] At last, if there is more than one periodic orbit, and considering that they are isolated, we should perform the calculation for each of them in the same way and sum their contributions at the end.

Let $(\bar{z}_0, \bar{s}_0)$ be a point on a contributing trajectory defined by $\bar{z}(t)$ and $\bar{s}(t)$. We call $\delta_\perp^2 F_0$ the second variation of $F$, around $(\bar{z}_0, \bar{s}_0)$ in the directions perpendicular to the direction of the propagation of the orbit. The contribution of this point to Eq. (23) can be written as

$$\frac{2j+1}{-4\pi^2}\sqrt{\frac{1}{\det \bar{M}_{bb}}}\frac{e^{(i/\hbar)\bar{F}}}{[1+|\bar{s}|^2]^2}\int e^{(i/2\hbar)\delta_\perp^2 \bar{F}_0} d[\delta u'_\perp]d[\delta v''_\perp]d[\delta U'_\perp]d[\delta V''_\perp], \tag{26}$$

where we have calculated the prefactor at $(\bar{z}_0, \bar{s}_0)$. The integral is over the hypersurface perpendicular to the direction of propagation of the orbit at $(\bar{z}_0, \bar{s}_0)$. To find the contribution of the whole orbit to (23) we should integrate over all its points. This is the reason why the expansion must be done in that specific direction, since contributions of adjacent points should not overlap.

In the next two subsections we construct an explicit canonical transformation to coordinates in these special directions.

### C. Expansion in an arbitrary direction

An arbitrary second order variation of the exponent $F$, around *a point* $(\bar{z}_0, \bar{s}_0)$ of the periodic orbit, can be written as

$$\delta^2 F = \delta \mathbf{v}^T (\nabla^2 \bar{F}) \delta \mathbf{v}, \tag{27}$$

where the bar indicates quantities calculated at the reference point and

$$\delta \mathbf{v}^T \equiv (u' - \bar{z}, U' - \bar{s}, v'' - \bar{z}^*, V'' - \bar{s}^*) \equiv (\delta u', \delta U', \delta v'', \delta V''),$$

$$\nabla^T \equiv (\partial/\partial u', \partial/\partial U', \partial/\partial v'', \partial/\partial V''), \tag{28}$$

where the upper index $T$ stands for the transpose. Assuming that $\mathcal{G}$ varies slowly when compared with $\mathcal{S}$ (Ref. 21) we write

$$\nabla^2 \bar{F} \approx \begin{pmatrix} \bar{\mathcal{S}}_{u'u'} & \bar{\mathcal{S}}_{u'U'} & \bar{\mathcal{S}}_{u'v''} + t_z & \bar{\mathcal{S}}_{u'V''} \\ \bar{\mathcal{S}}_{U'u'} & \bar{\mathcal{S}}_{U'U'} - t_s \bar{s}^{*2} & \bar{\mathcal{S}}_{U'v''} & \bar{\mathcal{S}}_{U'V''} + t_s \\ \bar{\mathcal{S}}_{v''u'} + t_z & \bar{\mathcal{S}}_{v''U'} & \bar{\mathcal{S}}_{v''v''} & \bar{\mathcal{S}}_{v''V''} \\ \bar{\mathcal{S}}_{V''u'} & \bar{\mathcal{S}}_{V''U'} + t_s & \bar{\mathcal{S}}_{V''v''} & \bar{\mathcal{S}}_{V''V''} - t_s s^2 \end{pmatrix}, \tag{29}$$

where $\bar{\mathcal{S}}_{\alpha\beta} \equiv \partial^2 \bar{\mathcal{S}}/\partial\alpha\partial\beta$, for $\alpha, \beta = u', U', v'', V''$. We have also defined

$$t_M \equiv \begin{pmatrix} t_z & 0 \\ 0 & t_s \end{pmatrix} = \begin{pmatrix} i\hbar & 0 \\ 0 & 2i\hbar j/(1+|\bar{s}|^2)^2 \end{pmatrix}. \tag{30}$$

According to Eq. (A4) in Appendix A, the second derivatives of the complex action $\mathcal{S}$ calculated at a given trajectory can be written in terms of its stability matrix $M$, defined by Eq. (19). Using Eq. (A4) we find

$$\nabla^2 \bar{F} = \begin{pmatrix} t_M(\bar{M}_{bb}^{-1}\bar{M}_{ba}) & t_M(\mathbf{1} - \bar{M}_{bb}^{-1}) \\ t_M(\mathbf{1} + \bar{M}_{ab}\bar{M}_{bb}^{-1}\bar{M}_{ba} - \bar{M}_{aa}) & t_M(-\bar{M}_{ab}\bar{M}_{bb}^{-1}) \end{pmatrix}. \tag{31}$$

Equations (27) and (31) give the second order expansion of $F$ around a point of a periodic orbit in an arbitrary direction in the space of variables $u'$, $U'$, $v''$, and $V''$.

### D. Special set of canonical variables

Since the vicinity of a periodic orbit is the only relevant part of the phase space in our problem, we can use a change of variables that is restricted to this region. We therefore introduce a new set of canonical variables $q$, $p$, $Q$, and $P$, assuming that $u=u(q,p)$, $v=v(q,p)$, $U=U(Q,P)$, $V=V(Q,P)$,[28] and that

$$\delta\mathbf{w} = \mathcal{T}\delta\mathbf{r}, \tag{32}$$

where

$$\delta\mathbf{w} \equiv \begin{pmatrix} \delta u \\ \delta U \\ \delta v \\ \delta V \end{pmatrix}, \quad \mathcal{T} \equiv \begin{pmatrix} \mathcal{T}_{aa} & \mathcal{T}_{ab} \\ \mathcal{T}_{ba} & \mathcal{T}_{bb} \end{pmatrix} \equiv \begin{pmatrix} t_{11} & 0 & t_{13} & 0 \\ 0 & t_{22} & 0 & t_{24} \\ t_{31} & 0 & t_{33} & 0 \\ 0 & t_{42} & 0 & t_{44} \end{pmatrix}, \quad \delta\mathbf{r} \equiv \begin{pmatrix} \delta q \\ \delta Q \\ \delta p \\ \delta P \end{pmatrix}. \tag{33}$$

According to these equations, we find the relations

$$t_{11} \equiv \frac{\partial u}{\partial q}, \quad t_{13} \equiv \frac{\partial u}{\partial p}, \quad t_{22} \equiv \frac{\partial U}{\partial Q}, \quad t_{24} \equiv \frac{\partial U}{\partial P},$$

$$t_{31} \equiv \frac{\partial v}{\partial q}, \quad t_{33} \equiv \frac{\partial v}{\partial p}, \quad t_{42} \equiv \frac{\partial V}{\partial Q}, \quad t_{44} \equiv \frac{\partial V}{\partial P}. \tag{34}$$

In addition, by inverting Eq. (32), we also find

$$\frac{t_{33}}{J_z} \equiv \frac{\partial q}{\partial u}, \quad -\frac{t_{31}}{J_z} \equiv \frac{\partial p}{\partial u}, \quad \frac{t_{44}}{J_s} \equiv \frac{\partial Q}{\partial U}, \quad -\frac{t_{42}}{J_s} \equiv \frac{\partial P}{\partial U},$$

$$-\frac{t_{13}}{J_z} \equiv \frac{\partial q}{\partial v}, \quad \frac{t_{11}}{J_z} \equiv \frac{\partial p}{\partial v}, \quad -\frac{t_{24}}{J_s} \equiv \frac{\partial Q}{\partial V}, \quad \frac{t_{22}}{J_s} \equiv \frac{\partial P}{\partial V}, \tag{35}$$

where $J_z \equiv t_{11}t_{33} - t_{13}t_{31}$ and $J_s \equiv t_{22}t_{44} - t_{24}t_{42}$. Notice that, since the periodic orbit is known, the elements $t_{ij}$ depend only on the transformation chosen. However, by demanding that $q$, $p$, $Q$, and $P$ be a set of canonical coordinates, we must impose

$$\dot{q} = \frac{\partial q}{\partial u}\dot{u} + \frac{\partial q}{\partial v}\dot{v} = \frac{1}{i\hbar}\{q,\tilde{H}\}_{uv} = \frac{1}{i\hbar}\{q,p\}_{uv}\frac{\partial \tilde{\mathrm{H}}}{\partial p} = \frac{\partial \tilde{\mathrm{H}}}{\partial p},$$

$$\dot{p} = \frac{\partial p}{\partial u}\dot{u} + \frac{\partial p}{\partial v}\dot{v} = \frac{1}{i\hbar}\{p,\widetilde{H}\}_{uv} = \frac{1}{i\hbar}\{q,p\}_{vu}\frac{\partial \widetilde{\mathrm{H}}}{\partial q} = -\frac{\partial \widetilde{\mathrm{H}}}{\partial q},$$

$$\dot{Q} = \frac{\partial Q}{\partial U}\dot{U} + \frac{\partial Q}{\partial V}\dot{V} = \frac{(1+UV)^2}{2ij\hbar}\{Q,\widetilde{H}\}_{UV} = \frac{(1+UV)^2}{2ij\hbar}\{Q,P\}_{UV}\frac{\partial \widetilde{\mathrm{H}}}{\partial P} = \frac{\partial \widetilde{\mathrm{H}}}{\partial P},$$

$$\dot{P} = \frac{\partial P}{\partial U}\dot{U} + \frac{\partial P}{\partial V}\dot{V} = \frac{(1+UV)^2}{2ij\hbar}\{P,\widetilde{H}\}_{UV} = \frac{(1+UV)^2}{2ij\hbar}\{Q,P\}_{VU}\frac{\partial \widetilde{\mathrm{H}}}{\partial Q} = -\frac{\partial \widetilde{\mathrm{H}}}{\partial Q}, \tag{36}$$

where $\widetilde{H}(q,Q,p,P) \equiv \widetilde{H}[u(q,p),U(Q,P),v(q,p),V(Q,P)]$. Equations (36) imply that

$$\{q,p\}_{uv} \equiv \mathcal{J}_z^{-1} = i\hbar \quad \text{and} \quad \{Q,P\}_{UV} \equiv \mathcal{J}_s^{-1} = \frac{2ij\hbar}{(1+UV)^2}. \tag{37}$$

Up to now we just introduce a general transformation from $(u,U,v,V)$ to the canonical set $(q,Q,p,P)$. However, our original problem, the solution of Eq. (21), involves the variables $(u,U)$, at the initial time, and $(v,V)$, at the final time. Therefore, we should write the vector $\delta\mathbf{v}$ of Eq. (27) in terms of the new variables. In order to do so, we write

$$\delta\mathbf{v} = \begin{pmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}\delta\mathbf{w}' + \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & 1 \end{pmatrix}\delta\mathbf{w}''. \tag{38}$$

Using Eq. (32), and also the stability matrix $\mathcal{M}$ in the new variables,

$$\delta\mathbf{r}'' = \mathcal{M}\,\delta\mathbf{r}' = \begin{pmatrix} \mathcal{M}_{aa} & \mathcal{M}_{ab} \\ \mathcal{M}_{ba} & \mathcal{M}_{bb} \end{pmatrix}\mathbf{r}', \tag{39}$$

we find

$$\delta\mathbf{v} = \mathcal{V}\delta\mathbf{y}, \tag{40}$$

where $\delta\mathbf{y}^T \equiv (\delta q', \delta Q', \delta p'', \delta P'')$ and

$$\mathcal{V} = \begin{pmatrix} \bar{\mathcal{T}}_{aa} - \bar{\mathcal{T}}_{ab}\bar{\mathcal{M}}_{bb}^{-1}\bar{\mathcal{M}}_{ba} & \bar{\mathcal{T}}_{ab}\bar{\mathcal{T}}_{bb}^{-1} \\ \bar{\mathcal{T}}_{ba}\bar{\mathcal{M}}_{aa} - \bar{\mathcal{T}}_{ba}\bar{\mathcal{M}}_{ab}\bar{\mathcal{M}}_{bb}^{-1}\bar{\mathcal{M}}_{ba} & \bar{\mathcal{T}}_{ba}\bar{\mathcal{M}}_{ab}\bar{\mathcal{M}}_{bb}^{-1} + \bar{\mathcal{T}}_{bb} \end{pmatrix}. \tag{41}$$

We should mention that Eq. (40) is valid only for deviations taken from periodic orbits, since we have assumed $\mathcal{T}' = \mathcal{T}'' = \bar{\mathcal{T}}$. This is also the reason why we have put the bar over $\mathcal{M}$. We can now fix the transformation $\mathcal{T}$ such that it corresponds to the set of coordinates, where the monodromy matrix $\bar{\mathcal{M}}$ assumes the simple form given by Eq. (B8) of Appendix B. The matrix $\mathcal{V}$ then becomes

$$\mathcal{V} = \begin{pmatrix} t_{11} & 0 & t_{13} & 0 \\ 0 & t_{22} & 0 & \lambda t_{24} \\ t_{31} & 0 & t_{33} - kt_{31} & 0 \\ 0 & \lambda t_{42} & 0 & t_{44} \end{pmatrix}, \tag{42}$$

whose determinant is $\lambda\widetilde{J}_z\widetilde{J}_s$ with $\widetilde{J}_s = t_{22}t_{44}\lambda' - t_{24}t_{42}\lambda$ and $\widetilde{J}_z = J_z - t_{11}t_{31}k$.

The matrix (42) defines the coordinate system where the integral of the second order variations shall be evaluated. According to this change of variables, using Eq. (B8) again, the matrix $\bar{M}$, which is written as $\bar{M} = \bar{\mathcal{T}}\bar{\mathcal{M}}\bar{\mathcal{T}}^{-1}$, becomes

$$\bar{M} = \begin{pmatrix} (J_z + t_{11}t_{31}k)/J_z & 0 & -t_{11}^2 k/J_z & 0 \\ 0 & (t_{22}t_{44}\lambda - t_{24}t_{42}\lambda')/J_s & 0 & -t_{22}t_{24}(\lambda-\lambda')/J_s \\ t_{31}^2 k/J_z & 0 & \tilde{J}_z/J_z & 0 \\ 0 & t_{42}t_{44}(\lambda-\lambda')/J_s & 0 & \tilde{J}_s/J_s \end{pmatrix}. \tag{43}$$

In these expressions $\lambda$ and $\lambda'$ are the two eigenvalues of $\bar{\mathcal{M}}$ that are not equal to 1 (but with $\lambda\lambda'=1$) and $k=\delta\tau/\delta E$. The last equation also enables us to write $\det \bar{M}_{bb}=(\tilde{J}_z\tilde{J}_s)/(J_zJ_s)$. Finally, we apply Eq. (43) directly to (31), finding

$$\nabla^2\bar{F} = \begin{pmatrix} t_{31}^2 k/J_z\tilde{J}_z & 0 & (\tilde{J}_z - J_z)/\tilde{J}_zJ_z & 0 \\ 0 & t_{42}t_{44}(\lambda-\lambda')/J_s\tilde{J}_s & 0 & (\tilde{J}_s - J_s)/\tilde{J}_sJ_s \\ (\tilde{J}_z - J_z)/\tilde{J}_zJ_z & 0 & t_{11}^2 k/J_z\tilde{J}_z & 0 \\ 0 & (\tilde{J}_s - J_s)/\tilde{J}_sJ_s & 0 & t_{24}t_{22}(\lambda-\lambda')/J_s\tilde{J}_s \end{pmatrix}. \tag{44}$$

Therefore, by defining $\delta\mathbf{v}^T(\nabla^2\bar{F})\delta\mathbf{v}=\delta\mathbf{y}^T\bar{\mathcal{F}}\delta\mathbf{y}$, we find

$$\mathcal{F} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & -t_{22}t_{42}(\lambda-1)^2/J_s & 0 & [(\lambda-1)/J_s](t_{24}t_{42}\lambda - t_{22}t_{44}) \\ 0 & 0 & (J_z'/J_z)k & 0 \\ 0 & [(\lambda-1)/J_s](t_{24}t_{42}\lambda - t_{22}t_{44}) & 0 & -t_{44}t_{24}(\lambda-1)^2/J_s \end{pmatrix}, \tag{45}$$

whose determinant of the $3\times 3$ non-null block is given by $D=-k(\tilde{J}_z\tilde{J}_s/J_zJ_s)\lambda(\lambda-1)^2$.

Now we use some results from Appendix B. The new deviations $\delta q$, $\delta Q$, and $\delta P$ are vectors that belong to the energy surface of the periodic orbit. The variable $q$, in particular, is the time of propagation, whereas a small displacement $\delta p$ gives origin to another periodic orbit belonging to the same family, but with slightly different energy and period. Equation (45) shows that $F$ does not change in the direction of $\delta q'$ as it should, since the action is constant along the orbit.

### E. Expansion around a periodic orbit: Evaluation

Using Eqs. (42), (43), and (45), we write the contribution of a *single* point $(\bar{z}^*,\bar{s}^*,\bar{z},\bar{s})$ of a periodic orbit to Eq. (23) as

$$\frac{(2j+1)\lambda}{8j\pi^2\hbar^2}\sqrt{\frac{\tilde{J}_z\tilde{J}_s}{J_zJ_s}}e^{(i/\hbar)\bar{F}}\int e^{(i/2\hbar)\delta\mathbf{y}^T\bar{\mathcal{F}}\delta\mathbf{y}}dQ'dp''dP'', \tag{46}$$

where the Gaussian integral can be solved directly resulting in $\sqrt{(2i\pi\hbar)^3/D}$. By performing the integral along the orbit, we find the contribution of the whole periodic orbit,

$$K_{\rm sc}(T) = \frac{2j+1}{4j\pi\hbar}\int\sqrt{\frac{2i\pi\hbar\lambda}{k(\lambda-1)^2}}e^{(i/\hbar)\bar{F}}dq', \tag{47}$$

where $F$, $k$, and $\lambda$ depend only on the periodic orbit and its period. Since $(\lambda-1)^2=\lambda\,\mathrm{tr}(\mathcal{M}-1)$, and both $\bar{F}$ and $\mathcal{M}$ are constant along the orbit, the last integral reduces to $\int dq'=T$, the primitive period of the orbit. The trace of the semiclassical propagator can finally be written as

$$K_{\rm sc}(T) = \frac{2j+1}{4j\pi\hbar}\sum_{\text{per.orb.}} T\sqrt{\frac{2i\pi\hbar}{k\,\mathrm{tr}(\mathcal{M}-1)}}e^{(i/\hbar)\bar{F}}. \tag{48}$$

### F. The Fourier transform

To find a semiclassical version of Eq. (3) we Fourier transform the trace (48),

$$g_{\rm sc}(E) \equiv \frac{1}{i\hbar}\int_0^\infty K_{\rm sc}(T)e^{(i/\hbar)ET}dT. \tag{49}$$

All periodic orbits, with all possible periods $T$ from 0 to $\infty$, should, in principle, be taken into account in the calculation of $g_{\rm sc}$. However, in the limit considered, such an integral can be solved again by the steepest descent method, according to which, among all values of $T$, the relevant contributions come from those close to $T=\tau$, satisfying the saddle point condition

$$-\left.\frac{\partial\mathcal{S}}{\partial T}\right|_{T=\tau} = \widetilde{H} = E, \tag{50}$$

where we used Eq. (20). This condition selects the values of $T=\tau\equiv\tau(E)$ for which trajectories have energy $E$. By considering, for simplicity, a single trajectory we obtain

$$g_{\rm sc}(E) = \frac{1}{i\hbar}\frac{2j+1}{4j\pi\hbar}\sqrt{\frac{2i\pi\hbar}{k\ \mathrm{tr}(\mathcal{M}-1)}}\tau e^{(i/\hbar)\bar{F}(\tau)+E\tau}\int e^{(i/2\hbar)\,(\partial^2\mathcal{S}/\partial T^2)|_\tau \delta T^2}d[\delta T]. \tag{51}$$

Using $(\partial^2\mathcal{S}/\partial T^2)|_\tau=-\partial E/\partial\tau=-k^{-1}$ the Gaussian integral gives $\sqrt{-2i\pi\hbar k}$. Also, since $(2j+1)/2j \to 1$ in the limit considered, we obtain

$$g_{\rm sc}(E) = \frac{1}{i\hbar}\sum_{\rm per.orb.}\frac{\tau e^{(i/\hbar)[S(E)+\mathcal{G}(E)]}}{\sqrt{\mathrm{tr}(\mathcal{M}-1)}}, \tag{52}$$

where Hamilton's action $S$ is the Legendre transform of the action $\mathcal{S}$ plus the normalization terms and it is explicitly given by

$$S(E) = \int_0^T\left\{\frac{i\hbar}{2}(\dot{u}v-\dot{v}u) - i\hbar j\left(\frac{U\dot{V}-V\dot{U}}{1+UV}\right)\right\}dt. \tag{53}$$

Notice that $\mathcal{G}$ contains the so-called Solari-Kochetov phase and also its counterpart for the canonical variables. Finally, using Eq. (5), we find

$$n(E) \approx \frac{1}{\pi\hbar}\sum_{\rm per.orb.}\frac{\tau\cos\{i/\hbar[S(E)+\mathcal{G}(E)]\}}{\sqrt{\mathrm{tr}(\mathcal{M}-1)}}, \tag{54}$$

as the analog of (6) for systems with spin. It can be directly compared with the result of Ref. 8, provided that the matrix $(\mathcal{M}-1)$ describes variations in terms of canonical variables. As usual, one has to be careful about the phase of the prefactor, adding the appropriate Maslov indices for each periodic orbit. The differences between the two formulas are related to the Hamiltonian function that generates the underlying classical dynamics, and the correction term $\mathcal{G}$. While in Ref. 8, the classical dynamics is governed by a function that includes the Weyl symbol of the canonical part of the Hamilton operator, and the average, in the basis $\{|s\rangle\}$, of the spin terms, in our work the dynamics is governed simply by $\langle z,s|\hat{H}|z,s\rangle$. On the other hand, our formula includes a kind of Solari-Kochetov phase for canonical variables in $\mathcal{G}$, which is not present in Ref. 8. As studied in Ref. 21, combining $\langle z|\hat{H}|z\rangle$ with the canonical part of $\mathcal{G}$, we recover the Weyl symbol of $\hat{H}$ for quadratic Hamiltonians, and, therefore, the work of Pletyukhov *et al.*

## VI. FINAL REMARKS

This paper, together with Ref. 12, presents a full and detailed derivation of the trace formula for general Hamiltonian systems with spin, starting from the quantum propagator. We have only treated the case of one spin and one canonical degrees of freedom, but extension to more dimensions is possible.[29,30]

Our final formula is slightly different from that of Ref. 8. It involves a correction similar to the Solari-Kochetov term for the canonical coherent states. Also, the underlying classical dynamics is governed by slightly different functions in each case. As discussed in Refs. 21, 31, and 32 different representations are possible for the canonical part of the propagator, involving different classical Hamiltonian functions and different correction terms that are added to the action in each case. The choice of Ref. 8 corresponds to the Weyl representation, whereas in this paper we have used the normal order, or $Q$ representation, of the Hamiltonian operator. For Hamiltonians involving up to quadratic terms in the canonical variables, it can be shown that the formulas coincide, the two differences canceling out each other. For Hamiltonians containing higher terms, a difference of order $\hbar^2$ appears.

Finally, we note that, in spite of being derived in the semiclassical limit, the trace formula should furnish good results even for spin-$\frac{1}{2}$ systems. The reason is that, in such a case, the interaction is linear in the spin variable, i.e., they involve only linear combinations of the generators of the algebra, which makes the approximation exact.[8,25]

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## APPENDIX A: TANGENT MATRIX AND DERIVATIVES OF THE ACTION

In this appendix, we derive a relation between the elements of the tangent matrix $M$, defined by Eq. (19), and the second derivatives of the complex action $\mathcal{S}(v'',V'',u',U',T)$, defined by Eq. (17). We begin by making variations on both sides of Eqs. (20), leading to

$$\left[\begin{pmatrix} s_{11} & s_{12} \\ s_{21} & s_{22} \end{pmatrix} + \begin{pmatrix} A & 0 \\ 0 & C \end{pmatrix}\right]\begin{pmatrix} \delta\mathbf{u}' \\ \delta\mathbf{v}'' \end{pmatrix} = \begin{pmatrix} 0 & B \\ D & 0 \end{pmatrix}\begin{pmatrix} \delta\mathbf{u}'' \\ \delta\mathbf{v}' \end{pmatrix}, \tag{A1}$$

where we have defined

$$\begin{pmatrix} s_{11} & s_{12} \\ s_{21} & s_{22} \end{pmatrix} \equiv \nabla^2\mathcal{S}, \quad \begin{pmatrix} A & B \\ D & C \end{pmatrix} \equiv \begin{pmatrix} 0 & 0 & -i\hbar & 0 \\ 0 & -2ij\hbar V'^2/(1+U'V')^2 & 0 & -2ij\hbar/(1+U'V')^2 \\ -i\hbar & 0 & 0 & 0 \\ 0 & -ij\hbar/(1+U''V'')^2 & 0 & -2ij\hbar U''^2/(1+U''V'')^2 \end{pmatrix}, \tag{A2}$$

the operator $\nabla^T \equiv (\partial/\partial u', \partial/\partial U', \partial/\partial v'', \partial/\partial V'')$ and $\delta\mathbf{u}^T \equiv (\delta u, \delta U)$, $\delta\mathbf{v}^T \equiv (\delta v, \delta V)$.

Rearranging Eq. (A1) in order to write the final displacements $\delta\mathbf{u}''$ and $\delta\mathbf{v}''$ as a function of the initial ones $\delta\mathbf{u}'$ and $\delta\mathbf{v}'$, we can relate the matrices $\nabla^2\mathcal{S}$ and $M$,

$$M = \begin{pmatrix} D^{-1}[s_{21} - (s_{22}+C)s_{12}^{-1}(s_{11}+A)] & D^{-1}(s_{22}+C)s_{12}^{-1}B \\ -s_{12}^{-1}(s_{11}+A) & s_{12}^{-1}B \end{pmatrix}, \tag{A3}$$

or, inverting the relation,

$$\nabla^2 \mathcal{S} = \begin{pmatrix} -BM_{bb}^{-1}M_{ba} - A & BM_{bb}^{-1} \\ D[M_{aa} - M_{ab}M_{bb}^{-1}M_{ba}] & DM_{ab}M_{bb}^{-1} - C \end{pmatrix}. \tag{A4}$$

For periodic trajectories the tangent matrix $M$ is the monodromy matrix and, according to Eq. (A2), $B=D$, since $U'=U''$ and $V'=V''$.

## APPENDIX B: STANDARD FORM OF THE MONODROMY MATRIX

The purpose of this appendix is to find a new set of coordinates in which the monodromy matrix $\mathcal{M}$ takes its simplest. We follow very closely the ideas presented by Baranger and de Aguiar in Ref. 33.

### 1. Preliminaries

We consider a classical system with two degrees of freedom and define the bra, or row vector, as $\langle \mathbf{x}| \equiv (x_1,x_2,x_3,x_4) \equiv (q_1,q_2,p_1,p_2)$, where the $q_i$'s and $p_i$'s are canonical variables. The transpose of $\langle \mathbf{x}|$ is denoted by the ket, or column vector, $|\mathbf{x}\rangle$. Notice that there is no complex conjugation in the transformation of a ket into a bra. All phase space variables are real at this point.

The $\mathcal{M}$ matrix propagates small initial displacements $|\delta\mathbf{x}'\rangle$ around a periodic orbit of period $\tau$, namely,

$$|\delta\mathbf{x}''\rangle = \mathcal{M}|\delta\mathbf{x}'\rangle, \tag{B1}$$

where a single (double) prime stands for the initial (final) time.

The symplectic property of $\mathcal{M}$ ensures that its eigenvalues occur in pairs whose product is 1.[34] In addition, for an initial displacement $|\delta\mathbf{x}'\rangle$ in the direction of the periodic trajectory, i.e., in the direction of $|\dot{\mathbf{x}}'\rangle$, we find $|\delta\mathbf{x}''\rangle = |\delta\mathbf{x}'\rangle$ after the time $\tau$. Combining these two arguments we assert that there exist two eigenvalues of $\mathcal{M}$ equal to 1. The other two are either

$$\lambda = e^{i\alpha}, \quad \lambda' = e^{-i\alpha} \quad \text{(for stable orbits)},$$

or

$$\lambda = \pm e^{\beta}, \quad \lambda' = \pm e^{-\beta} \quad \text{(for unstable orbits)}. \tag{B2}$$

Each of the latter two eigenvalues has a distinct eigenvector. The two unit eigenvalues, on the other hand, have only one eigenvector, which we call *the sliding vector* $|\mathbf{l}\rangle$, since it displaces the trajectory by sliding it along itself.

The discussion above enables us to make use of three vectors to set up our new basis,

$$|\mathbf{w_1}\rangle \equiv |\mathbf{l}\rangle,$$

$$|\mathbf{w}_2\rangle \equiv \text{eigenvector of } \mathcal{M} \text{ for eigenvalue } \lambda,$$

$$|\mathbf{w}_4\rangle \equiv \text{eigenvector of } \mathcal{M} \text{ for eigenvalue } \lambda' = \lambda^{-1}. \tag{B3}$$

As we have only three distinct eigenvectors of $\mathcal{M}$, we need a fourth special vector $|\mathbf{w}_3\rangle$, which is not an eigenvector of $\mathcal{M}$. As we shall see toward the end of this appendix, for a given starting point of the periodic trajectory, displacements in the direction of the vectors $|\mathbf{w}_1\rangle$, $|\mathbf{w}_2\rangle$, and $|\mathbf{w}_4\rangle$ span the energy surface. Therefore, our choice for $|\mathbf{w}_3\rangle$ is a vector which take us from the origin of our periodic trajectory to a point on a neighboring periodic trajectory of the same family, with a slightly different $\tau$ and a slightly different $E$. Such a vector is easily constructed in pratice of course, since it should come directly out of the numerical calculations of the family of periodic trajectories. In the following, we shall construct this vector in theory. We call it *the family vector* and we denote it by $|\mathbf{r}\rangle$.

### 2. The family vector

Given $|\mathbf{x}'\rangle$ at time 0, Hamilton equations allow us to calculate $|\mathbf{x}''\rangle$ at time $t$. This can be written as $x_i''=F_i(\mathbf{x}',t)$, for $i=1,2,3,4$. A small variation in $|\mathbf{x}'\rangle$ and in $t$ leads to a small variation in $|\mathbf{x}''\rangle$,

$$\delta x_i'' = \sum_j \frac{\partial F_i}{\partial x_j'}\delta x_j' + \frac{\partial F_i}{\partial t}\delta t. \tag{B4}$$

As we are working with a periodic orbit of period $\tau$, we may identify the function $\partial F_i/\partial x_j$ at $t=\tau$ as the element $\mathcal{M}_{ij}$ of the monodromy matrix. Besides, the vector whose components are the functions $\partial F_i/\partial t=\dot{x}_i(t)$, also calculated at $t=\tau$, is proportional to the sliding vector $|\mathbf{l}\rangle$.

Concerning the family vector, due to its definition, to find it we must impose that the final displacement $|\delta\mathbf{x}''\rangle$ at a time $t=\tau+\delta\tau$ be equal to the initial one $|\delta\mathbf{x}'\rangle$. Setting $|\delta\mathbf{x}'\rangle=|\delta\mathbf{x}''\rangle=|\delta\mathbf{x}\rangle$, we have

$$|\delta\mathbf{x}\rangle = \mathcal{M}|\delta\mathbf{x}\rangle + k|\mathbf{l}\rangle\delta\tau \Rightarrow (\mathbf{1}-\mathcal{M})|\mathbf{r}\rangle = k|\mathbf{l}\rangle, \tag{B5}$$

where we have identified the family vector as $|\mathbf{r}\rangle=|\delta\mathbf{x}\rangle/\delta\tau$. The proportionality coefficient $k$ will be treated later.

In Eq. (B5), as the matrix $(\mathcal{M}-\mathbf{1})$ is singular, we must find the conditions for the existence of a solution for $|\mathbf{r}\rangle$. From the symplectic relation

$$\mathcal{M}^{-1} = J\mathcal{M}^T J^{-1},$$

where

$$J = \begin{pmatrix} 0 & \mathbf{1} \\ -\mathbf{1} & 0 \end{pmatrix}, \tag{B6}$$

we find that because $\mathcal{M}^{-1}|\mathbf{l}\rangle=|\mathbf{l}\rangle$, then $\langle\mathbf{l}|J\mathcal{M}=\langle\mathbf{l}|J$. In other words, the left eigenvector of $\mathcal{M}$ with eigenvalue of 1 is $\langle\mathbf{l}|J$. Applying it to Eq. (B5), we find the condition $\langle\mathbf{l}|J|\mathbf{l}\rangle=0$. Since this condition is satisfied by any vector, a solution for $|\mathbf{r}\rangle$ exists.

Finally, since $|\mathbf{w}_3\rangle\equiv|\mathbf{r}\rangle$, the three eigenvalue relations, plus Eq. (B5), furnish

$$\mathcal{M}|\mathbf{w}_1\rangle = |\mathbf{w}_1\rangle, \quad \mathcal{M}|\mathbf{w}_3\rangle = |\mathbf{w}_3\rangle - k|\mathbf{w}_1\rangle,$$

$$\mathcal{M}|\mathbf{w}_2\rangle = \lambda|\mathbf{w}_2\rangle, \quad \mathcal{M}|\mathbf{w}_4\rangle = \lambda'|\mathbf{w}_4\rangle, \tag{B7}$$

so that, in this basis, $\mathcal{M}$ has the simple form

$$\mathcal{M} = \begin{pmatrix} 1 & 0 & -k & 0 \\ 0 & \lambda & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & \lambda' \end{pmatrix}, \tag{B8}$$

which is called *the standard form of* $\mathcal{M}$.[33]

Quoting Ref. 33, "We shall have much more calculating power, however, if we can deal with bilinear forms, i.e., with bras as well as kets, and if we avail ourselves of the special metric engendered by the symplectic relation." This is done next.

### 3. The bra vectors

In this section we shall construct four bra vectors $\langle\mathbf{y}_i|$ such that $\langle\mathbf{y}_i|\mathbf{w}_j\rangle=\delta_{ij}$ and, therefore, $\Sigma_i|\mathbf{w}_i\rangle\langle\mathbf{y}_i|=\mathbf{1}$. The bra vectors allow us to write the standard form as $\langle\mathbf{y}_i|\mathcal{M}|\mathbf{w}_j\rangle$ and

$$\mathcal{M} = |\mathbf{w}_1\rangle\langle\mathbf{y}_1| - k|\mathbf{w}_1\rangle\langle\mathbf{y}_3| + |\mathbf{w}_3\rangle\langle\mathbf{y}_3| + \lambda|\mathbf{w}_2\rangle\langle\mathbf{y}_2| + \lambda'|\mathbf{w}_4\rangle\langle\mathbf{y}_4|. \tag{B9}$$

From this we see that

$$\langle\mathbf{y}_1|\mathcal{M} = \langle\mathbf{y}_1| - k\langle\mathbf{y}_3|, \quad \langle\mathbf{y}_3|\mathcal{M} = \langle\mathbf{y}_3|,$$

$$\langle\mathbf{y}_2|\mathcal{M} = \lambda\langle\mathbf{y}_2|, \quad \langle\mathbf{y}_4|\mathcal{M} = \lambda'\langle\mathbf{y}_4|, \tag{B10}$$

which means that $\langle\mathbf{y}_2|$, $\langle\mathbf{y}_3|$, and $\langle\mathbf{y}_4|$ are left eigenvectors of $\mathcal{M}$.

To determine the $\langle\mathbf{y}_i|$'s, we return to the sympletic property of $\mathcal{M}$, according to which, if $\mathcal{M}|\mathbf{w}\rangle=\mu|\mathbf{w}\rangle$, then $\mathcal{M}^{-1}|\mathbf{w}\rangle=\mu^{-1}|\mathbf{w}\rangle$, and, consequently, $\langle\mathbf{w}|J\mathcal{M}=\mu^{-1}\langle\mathbf{w}|J$. In other words, if $|\mathbf{w}\rangle$ is right eigenvector for the eigenvalue $\mu$, then $\langle\mathbf{w}|J$ is left eigenvector with eigenvalue $\mu^{-1}$. Therefore, we are able to identify three left eigenvectors of $\mathcal{M}$: $\langle\mathbf{w}_1|J$, $\langle\mathbf{w}_2|J$, and $\langle\mathbf{w}_4|J$, with eigenvalues 1, $\lambda^{-1}$, and $\lambda'^{-1}$, respectively. Comparing with Eq. (B10), we find

$$\langle\mathbf{y}_3| = k_3\langle\mathbf{w}_1|J, \quad \langle\mathbf{y}_2| = k_2\langle\mathbf{w}_4|J, \quad \langle\mathbf{y}_4| = k_4\langle\mathbf{w}_2|J, \tag{B11}$$

where the proportionality constants $k_2$, $k_3$, and $k_4$ may be determined by the normalization $\langle\mathbf{y}_i|\mathbf{w}_j\rangle=\delta_{ij}$: $k_4=-k_2=\langle\mathbf{w}_2|J|\mathbf{w}_4\rangle^{-1}$ and $k_3=\langle\mathbf{w}_1|J|\mathbf{w}_3\rangle^{-1}$.

We still have to find $\langle\mathbf{y}_1|$. We start from

$$\mathcal{M}|\mathbf{w}_3\rangle = |\mathbf{w}_3\rangle - k|\mathbf{w}_1\rangle \Rightarrow k_3\langle\mathbf{w}_3|J(\mathcal{M}-1) = k\langle\mathbf{y}_3|. \tag{B12}$$

By comparing it with the first of Eqs. (B10) we find $\langle\mathbf{y}_1|=-k_3\langle\mathbf{w}_3|J+\alpha\langle\mathbf{y}_3|$, where the factor $\alpha$ is an unknown factor. Recall that this uncertainty is due to the fact that the matrix $(\mathcal{M}-1)$ is singular and $\langle\mathbf{y}_3|$ is a left solution of the homogenous equation. We determine $\alpha$ by writing $\langle\mathbf{y}_1|\mathbf{w}_3\rangle=0$, which yields $\alpha=0$. Hence

$$\langle\mathbf{y}_1| = -k_3\langle\mathbf{w}_3|J, \quad \langle\mathbf{y}_3| = k_3\langle\mathbf{w}_1|J,$$

$$\langle\mathbf{y}_2| = -k_4\langle\mathbf{w}_4|J, \quad \langle\mathbf{y}_4| = k_4\langle\mathbf{w}_2|J. \tag{B13}$$

### 4. New coordinate system as a set of canonical variables

We have now a new coordinate system, valid for infinitesimal displacements in the vicinity of the origin chosen on the periodic trajectory, and such that in this new system the matrix $\mathcal{M}$ takes the standard form (B8). We want to demand one more thing: we would like the new coordinates to form a canonical set of variables.

In order to write this, let us define a vector containing the four new coordinates $Q_1$, $Q_2$, $P_1$, and $P_2$ by

$$\begin{pmatrix} q_1 \\ q_2 \\ p_1 \\ p_2 \end{pmatrix} = C\begin{pmatrix} Q_1 \\ Q_2 \\ P_1 \\ P_2 \end{pmatrix} \equiv \begin{pmatrix} w_1^{(1)} & w_2^{(1)} & w_3^{(1)} & w_4^{(1)} \\ w_1^{(2)} & w_2^{(2)} & w_3^{(2)} & w_4^{(2)} \\ w_1^{(3)} & w_2^{(3)} & w_3^{(3)} & w_4^{(3)} \\ w_1^{(4)} & w_2^{(4)} & w_3^{(4)} & w_4^{(4)} \end{pmatrix}\begin{pmatrix} Q_1 \\ Q_2 \\ P_1 \\ P_2 \end{pmatrix}, \tag{B14}$$

where $w_j^{(i)}$ is the component of the $i$th line of $|\mathbf{w}_j\rangle$. We want the transformation matrix $C$ to be sympletic, i.e., $C^{-1}=JC^TJ^{-1}$, which can also be written as $C^TJC=J$. Performing the calculation, we have

$$C^T J C = \begin{pmatrix} \langle \mathbf{w}_1|J|\mathbf{w}_1\rangle & \langle \mathbf{w}_1|J|\mathbf{w}_2\rangle & \langle \mathbf{w}_1|J|\mathbf{w}_3\rangle & \langle \mathbf{w}_1|J|\mathbf{w}_4\rangle \\ \langle \mathbf{w}_2|J|\mathbf{w}_1\rangle & \langle \mathbf{w}_2|J|\mathbf{w}_2\rangle & \langle \mathbf{w}_2|J|\mathbf{w}_3\rangle & \langle \mathbf{w}_2|J|\mathbf{w}_4\rangle \\ \langle \mathbf{w}_3|J|\mathbf{w}_1\rangle & \langle \mathbf{w}_3|J|\mathbf{w}_2\rangle & \langle \mathbf{w}_3|J|\mathbf{w}_3\rangle & \langle \mathbf{w}_3|J|\mathbf{w}_4\rangle \\ \langle \mathbf{w}_4|J|\mathbf{w}_1\rangle & \langle \mathbf{w}_4|J|\mathbf{w}_2\rangle & \langle \mathbf{w}_4|J|\mathbf{w}_3\rangle & \langle \mathbf{w}_4|J|\mathbf{w}_4\rangle \end{pmatrix} = J, \tag{B15}$$

implying that, for $i \leqslant j$,

$$\langle \mathbf{w}_i|J|\mathbf{w}_j\rangle = \begin{cases} 1, & \text{for } (i,j)=(1,3) \text{ or } (i,j)=(2,4) \\ 0, & \text{otherwise.} \end{cases} \tag{B16}$$

The second condition is automatically satisfied by our vectors, and the first one, a kind of normalization condition, imposes that $k_3$ and $k_4$ must be 1.

Now it should be possible to determine the value of the coefficient $k$, which figures in the standard form of the $\mathcal{M}$ matrix. To do this, we calculate the change in energy $\delta E$ associated with $|\delta \mathbf{x}\rangle$,

$$\delta E = \sum_i \frac{\partial H}{\partial x_i}\delta x_i = \dot{q}_1 \delta p_1 + \dot{q}_2 \delta p_2 - \dot{p}_1 \delta q_1 - \dot{p}_2 \delta q_2 = \langle \dot{\mathbf{x}}|J|\delta \mathbf{x}\rangle. \tag{B17}$$

Recalling the definition of $|\mathbf{r}\rangle \equiv |\delta \mathbf{x}\rangle / \delta\tau$ and of $|\mathbf{l}\rangle \equiv k|\dot{\mathbf{x}}\rangle$, we see that

$$\delta E = \frac{\delta\tau}{k}\langle \mathbf{l}|J|\mathbf{r}\rangle = \frac{\delta\tau}{k}\langle \mathbf{w}_1|J|\mathbf{w}_3\rangle \Rightarrow k = \frac{\delta\tau}{\delta E} = \frac{d\tau}{dE}. \tag{B18}$$

Referring back to the coordinates $(Q_1, Q_2, P_1, P_2)$, we see that $Q_1$ is the time for displacements along the trajectory and $P_1$ is the energy for displacements away from the trajectory in the plane of the "family." Finally, Eq. (B17) shows us that the energy shell contains all vectors $|\mathbf{d}\rangle$ such that $\langle \mathbf{l}|J|\mathbf{d}\rangle = 0$. Therefore $|\mathbf{l}\rangle$, $|\mathbf{w}_2\rangle$, and $|\mathbf{w}_4\rangle$ span the energy shell.


[1] L. D. Landau and E. M. Lifshitz, *Quantum Mechanics: Non-Relativistic Theory* (Pergamon, London, 1977).
[2] A. Einstein, Verh. Dtsch. Phys. Ges. **19**, 82 (1917); J. B. Keller, Ann. Phys. (N.Y.) **4**, 180 (1958).
[3] M. C. Gutzwiller, *Chaos in Classical and Quantum Mechanics* (Springer-Verlag, New York, 1990); J. Math. Phys. **8**, 1979 (1967); **10**, 1004 (1969); **11**, 1791 (1970); **12**, 343 (1971).
[4] C. Amann and M. Brack, J. Phys. A **35**, 6009 (2002).
[5] R. G. Littlejohn and W. G. Flynn, Phys. Rev. A **44**, 5239 (1991); **45**, 7697 (1992).
[6] H. Frisk and T. Guhr, Ann. Phys. (N.Y.) **221**, 229 (1993).
[7] J. Bolte and S. Keppeler, Phys. Rev. Lett. **81**, 1987 (1998); Ann. Phys. (N.Y.) **274**, 125 (1999).
[8] M. Pletyukhov, Ch. Amann, M. Mehta, and M. Brack, Phys. Rev. Lett. **89**, 116601 (2002); M. Pletyukhov and O. Zaitsev, J. Phys. A **36**, 5181 (2003); O. Zaitsev, *ibid.* **35**, L721 (2002).
[9] A. Garg and M. Stone, Phys. Rev. Lett. **92**, 010401 (2004); M. Novaes and M. A. M. de Aguiar, Phys. Rev. A **71**, 012104 (2005).
[10] A. J. Leggett, S. Chakravarty, A. T. Dorsey, M. P. A. Fisher, A. Garg, and W. Zwerger, Rev. Mod. Phys. **59**, 1 (1987).
[11] E. Martin-Fierro and E. Pollak, J. Chem. Phys. **126**, 164108 (2007).
[12] A. D. Ribeiro, M. A. M. de Aguiar, and A. F. R. de Toledo Piza, J. Phys. A **39**, 3085 (2006).
[13] A. Sugita, Ann. Phys. (N.Y.) **288**, 277 (2001).
[14] J. R. Klauder and B. S. Skagerstan, *Coherent States. Applications in Physics and Mathematical Physics* (World Scientific, Singapore, 1985).
[15] A. Perelomov, *Generalized Coherent States and their Applications* (Springer-Verlag, Berlin, 1986).
[16] W. M. Zhang, D. H. Feng, and R. Gilmore, Rev. Mod. Phys. **62**, 867 (1990).
[17] E. Schröedinger, Proceedings of the Prussian Academy of Sciences XIX, pp. 296–303 (1930), in *Erwin Schrödinger, Gesammelte Abhandlungen*, Band 3, Verlag der Österreichschen Akkademie der Wissenschaften, Wien, pp. 348–356 (1984).
[18] J. R. Klauder, in *Continuous Representations and Path Integrals, Revisited*, edited by G. J. Papadopoulos and J. T. Devreese, NATO Advanced Study Institute, Series B: Physics (Plenum, New York, 1978).
[19] J. R. Klauder, Phys. Rev. D **19**, 2349 (1979).
[20] E. A. Kochetov, J. Phys. A **31**, 4473 (1998).
[21] M. Baranger, M. A. M. de Aguiar, F. Keck, H. J. Korsch, and B. Schellaaß, J. Phys. A **34**, 7227 (2001).
[22] D. V. Shalashilin and M. S. Child, Chem. Phys. **304**, 103 (2004).
[23] H. Solari, J. Math. Phys. **28**, 1097 (1987).
[24] V. R. Vieira and P. D. Sacramento, Nucl. Phys. B **448**, 331 (1995).

[25] E. A. Kochetov, J. Math. Phys. **36**, 4667 (1995).
[26] M. Stone, K.-S. Park, and A. Garg, J. Math. Phys. **41**, 8025 (2000).
[27] A. Alscher and H. Grabert, Eur. Phys. J. D **14**, 127 (2001); X. Song and T. Van Voorhis, J. Chem. Phys. **124**, 134104 (2006).
[28] M. A. M. de Aguiar, K. Furuya, C. H. Lewenkopf, and M. C. Nemes, Ann. Phys. (N.Y.) **216**, 291 (1992).
[29] A. D. Ribeiro, M. A. M. de Aguiar, and M. Baranger, Phys. Rev. E **69**, 066204 (2004).
[30] C. Braun and A. Garg, J. Math. Phys. **48**, 032104 (2007).
[31] L. C. dos Santos and M. A. M. de Aguiar, J. Phys. A **39**, 13465 (2006).
[32] E. Martin-Fierro and J. M. Gomez Llorente, Chem. Phys. **322**, 13 (2006).
[33] M. Baranger and M. A. M. de Aguiar (unpublished).
[34] V. I. Arnold, *Mathematical Methods of Classical Mechanics* (Springer, New York, 1978).